

# Quantum Critical Metals: beyond the Order Parameter Fluctuations

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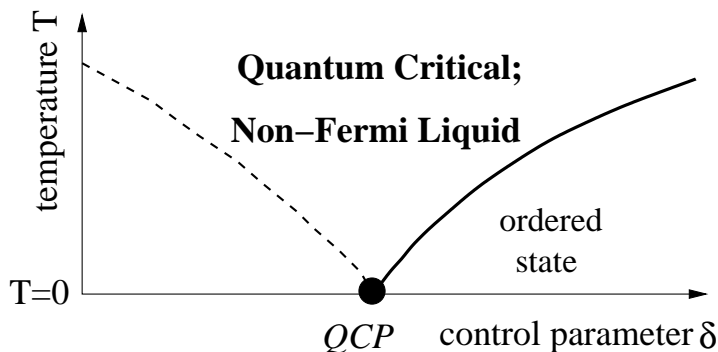
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**Abstract.** The standard description of quantum critical points takes into account only fluctuations of the order parameter, and treats quantum fluctuations as extra dimensions of classical fluctuations. This picture can break down in a qualitative fashion in quantum critical metals: non-Fermi liquid electronic excitations are formed precisely at the quantum critical point and appear as a part of the quantum-critical spectrum. In the case of heavy fermion metals, it has been proposed that the non-Fermi liquid behavior is characterized by the destruction of the Kondo effect. The latter invalidates Hertz's Gaussian theory of paramagnons and leads to an interacting theory that is "locally quantum critical". We summarize the theoretical and experimental developments on the subject. We also discuss their broader implications, and make contact with recent work on quantum critical magnets.

## 1 The Order Parameter Fluctuation Theory of Quantum Critical Points and its Breakdown

Phase transitions come in different varieties. Generically, they are characterized by the onset of an order parameter. A classical critical point, occurring at a finite temperature phase transition of second-order, is described in terms of a coarse-grained theory of spatial, but time-independent, fluctuations of the order parameter [1]. Such a description also serves as the basis to categorize the universality classes of critical points. Quantum critical points (QCPs) take place at zero temperature. They differ from their classical counterparts in that the static (classical) and dynamic (quantum) fluctuations are mixed and both have to be incorporated in the critical theory. It is, however, standard to assume that they too can be described in terms of fluctuations of the order parameter: the only distinction being that the fluctuations are not only in space but also in (imaginary) time [2,3].

It has been realized over the past few years that this picture can break down in a qualitative fashion in quantum critical metals [4,5]. Non-Fermi liquid excitations emerge precisely at the QCP, and they need to be kept as a part of the quantum-critical spectrum. This is illustrated in Fig. 1. On the one hand, quantum criticality is the mechanism for the non-Fermi liquid behavior. On the other hand, the non-Fermi liquid excitations feed back and change the universality class of the underlying QCP. The experimental motivations have largely come from heavy fermion QCPs [6,4,5]. Discussions of a similar spirit can be found in an earlier pedagogical article [7].



**Fig. 1.** Schematics of quantum phase transitions in strongly correlated metals. Quantum criticality leads to non-Fermi liquid excitations which, in turn, become a part of the quantum-critical spectrum and give rise to new types of quantum-critical point.

The notion that quantum fluctuations at a second-order zero-temperature phase transition amount to adding extra dimensions of purely classical fluctuations dates back to the work on the Ising model in a transverse field [8,3]. Within the renormalization group framework, Hertz [2] carried out such a mapping for a model of a metal undergoing a quantum spin-density-wave (SDW) transition. He showed that the number of the extra dimensions is equal to the dynamic exponent  $z$ . The result [2,9] is a  $d_{eff} = d + z$  (where  $d$  is the spatial dimensionality) dimensional critical theory of paramagnons [10,11,12,13]. It was not until recent years that quantum critical metals became experimentally realized, mostly in heavy fermion metals. In many cases, the experiments contradict the Hertz picture [6,4,5] (see below).

From a theoretical point of view, the possible breakdown of this picture can be seen in a number of ways. First, the construction of the order parameter fluctuation theory proceeds by integrating out fermions altogether. However, non-Fermi liquid excitations emerge exactly at the QCP (Fig. 1); they go away inside the phases on both sides of the QCP. These emergent excitations should be considered as a part of the quantum-critical spectrum. The resulting critical theory is then more than just fluctuations of the order parameter.

Second, in the mapping of quantum fluctuations into extra dimensions of classical fluctuations, one writes the partition function of a quantum mechanical system in terms of a summation over configurations of classical variables in space and time:

$$Z \sim \sum_{\text{config in } (\mathbf{x}, \tau)} Z(\text{config}). \quad (1)$$

However, if the partition function for the individual configurations in space and time is not positive semidefinite, Eq. (1) would not necessarily corre-

spond to a classical statistical mechanical theory in  $d + z$  dimensions. For electronic systems, this has been known through the “fermion sign problem” encountered in quantum Monte-Carlo methods [14]. The sign problem also appears in quantum spin systems. Indeed, recent work has demonstrated its effect in QCPs of two-dimensional quantum magnets [15] (see below).

## 2 Quantum Critical Heavy Fermions

Quantum criticality is of particular interest to the physics of strongly correlated metals. It provides a route towards non-Fermi liquid behavior [16,17], and may also serve as a means of generating collective states such as unconventional superconductors [18,19]. Heavy fermions have been playing an especially important role, for the simple reason that here QCPs have been explicitly identified [6].

The contradiction to the paramagnon description was initially found in the inelastic neutron scattering experiments of heavy fermion metals near an antiferromagnetic QCP [20,21,22]. The prediction of the paramagnon theory is straightforward. Due to Landau damping, the dynamic exponent  $z = 2$  in the antiferromagnetic case. The effective dimensionality of the fluctuations of the paramagnons,  $d_{\text{eff}} = d + 2$ , is either larger than or equal [21] to 4, the upper critical dimension. The fixed point is Gaussian, and the frequency dependence of the dynamical spin susceptibility is simply given by the Landau damping [2], with an exponent 1. At the same time, its temperature dependence is controlled by the quartic coupling among paramagnons; this coupling is dangerously irrelevant and produces a temperature exponent that is larger than 1 [9]. An important corollary is that the dynamical spin susceptibility necessarily violates  $\omega/T$  scaling [3]. (In special cases, integrating out fermions within the Hertz framework makes the coupling constants of the paramagnon theory non-analytic [23,24]. Such effects may lead to fractional exponents in the dynamical spin susceptibility at  $\mathbf{q} \sim \mathbf{Q}$ , but not  $\omega/T$  scaling [24].)

The experiments [20,21,22], on the other hand, observe  $\omega/T$  scaling. Moreover, the critical exponent for the frequency and temperature dependences is fractional. Finally, this same fractional exponent is observed even at wavevectors far away from the antiferromagnetic ordering wavevector  $\mathbf{Q}$ , in a form [20]

$$\chi(\mathbf{q}, \omega) = \frac{\text{const.}}{f(\mathbf{q}) + (-i\omega)^\alpha W(\omega/T)}, \quad (2)$$

where  $f(\mathbf{q})$  vanishes as  $\mathbf{q}$  approaches the antiferromagnetic wavevector  $\mathbf{Q}$  and stays non-zero elsewhere. The fact that this same fractional exponent  $\alpha$  appears essentially everywhere in the Brillouin zone suggests that its origin is local, as noted in Ref. [20].

Heavy fermions near a magnetic quantum phase transition should be well-described in terms of a Kondo lattice model:

$$\mathcal{H} = \sum_{ij, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i J_K \mathbf{S}_i \cdot \mathbf{s}_{c,i} + \sum_{ij} I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (3)$$

We are considering metallic systems, away from half-filling (*i.e.*, the number of conduction electrons is other than one per  $f$  electron). We can define the tuning parameter of this model as  $\delta$ , the ratio of the RKKY interaction to the bare Kondo scale  $T_K^0$ . For negligible  $\delta$ , the Kondo effect dominates [25,26]: the local moments are quenched and the excitations below some energy scale,  $E_{\text{loc}}^*$ , are spin- $\frac{1}{2}$  and charge- $e$  Kondo resonances [27]. The result is a paramagnetic heavy fermion metal. For large  $\delta$ , on the other hand, the interactions between the local moments play the dominant role. For dimensions higher than one and in the absence of strong geometrical frustration, the ground state is expected to be magnetically ordered. Typically, this would be an antiferromagnetic metal (as can be expected when the system is not too far away from half-filling).

What is the nature of the quantum phase transitions? It was suggested in Ref. [28] that the behavior of  $E_{\text{loc}}^*$  can be used as a characterization. As defined earlier, this is the scale below which local-moments are turned into Kondo resonances. It can also be operationally defined in terms of the spin damping or “spin self-energy”  $M(\omega)$  (see below):  $E_{\text{loc}}^*$  separates the region ( $\omega \gg E_{\text{loc}}^*$ ) where  $M(\omega)$  contains a fractional exponent and that ( $\omega \ll E_{\text{loc}}^*$ ) where it is linear in frequency. Two different classes of QCP occur depending on whether  $E_{\text{loc}}^*$  stays finite or vanishes at the QCP [28]. Subsequent microscopic works [4,29,30,31] have indeed shown such QCPs. Related approaches have also been developed in Refs. [32,5,33].

### 3 Microscopic Results and Their Robustness

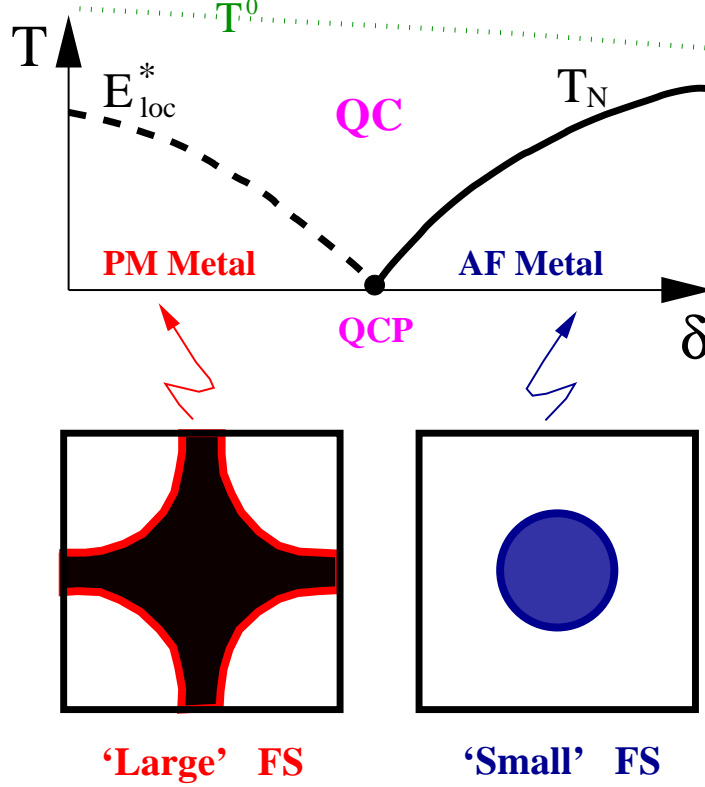
#### 3.1 Microscopic Results

The microscopic analysis was carried out within the extended dynamical mean field theory of Kondo lattice systems [29,34] (this approach goes beyond the dynamical mean field theory [35,36]; for the initial development of the method, see Refs. [37,38]). In this approach, the spin spin-energy is taken to be momentum-independent, which is expected to be valid for antiferromagnetic quantum critical metals provided the spatial anomalous dimension  $\eta = 0$ .

The “local quantum critical point” arises in this microscopic approach to the Kondo lattice model. The Kondo coupling is relevant in the renormalization group sense on the paramagnetic side, leading to Kondo singlet formation and Kondo resonances below a finite energy scale  $E_{\text{loc}}^*$ . At the QCP, however, the Kondo coupling is on the verge of becoming irrelevant. So  $E_{\text{loc}}^*$  goes to zero precisely at the QCP; see Fig. 2.

The microscopic result also provides yet another alternative means to define  $E_{\text{loc}}^*$ , which appears as an infrared cutoff scale in the local spin susceptibility,  $\chi_{\text{loc}} \equiv \langle \chi(\mathbf{q}, \omega) \rangle_{\mathbf{q}}$ . On the paramagnetic metal side,  $E_{\text{loc}}^*$  is finite, and  $\chi_{\text{loc}}$  has the Pauli behavior reflecting the Kondo resonances. At the QCP, on the other hand,  $E_{\text{loc}}^* = 0$  and  $\chi_{\text{loc}}$  is singular. The singularity is however

weaker than the Curie behavior in the non-scaling regime above the ultraviolet cutoff scale  $T^0$ . ( $T^0$  is of the order of the single-ion Kondo temperature  $T_K^0$ , and is always finite.)



**Fig. 2.** Local quantum critical point. The Fermi surface undergoes a sudden reconstruction across the QCP; within the paramagnetic Brillouin zone, it is ‘large’ on the heavy fermion side and ‘small’ on the antiferromagnetic side.

The initial analytic result for the quantum-critical dynamics was derived with the aid of an  $\epsilon$ -expansion of the self-consistent Bose-Fermi Kondo model [4,29]. The local spin susceptibility is

$$\chi_{\text{loc}}(\omega, T = 0) = \frac{1}{2\Lambda} \ln \frac{\Lambda}{-i\omega}, \quad (4)$$

where the energy scale  $\Lambda \approx T_K^0$ . The corresponding spin self-energy has the form

$$M(\omega, T) \approx -I_{\mathbf{Q}} + A (-i\omega)^\alpha W\left(\frac{\omega}{T}\right), \quad (5)$$

and the exponent is

$$\alpha = \frac{1}{2\rho_I(I_{\mathbf{Q}})\Lambda}. \quad (6)$$

Since the product  $\rho_I(I_{\mathbf{Q}})\Lambda$  is expected to be of order unity at the transition [4,29],  $\alpha$  should be fractional.

The singular fluctuations seen in the local susceptibility reflects the embedding of the criticality of the local Kondo physics in the criticality associated with the antiferromagnetic ordering. The singular form might raise the concern that the local quantum critical point is pre-empted by magnetic ordering, which would turn the transition first order. It was argued that a second order transition is natural: for two-dimensional magnetic fluctuations, a divergent local susceptibility necessarily accompanies a divergent peak susceptibility (provided the spatial anomalous dimension  $\eta = 0$ , which is to be expected at the quantum transition [29]).

This issue has been further addressed numerically [30]. We've considered the model with Ising anisotropy, the case with a maximum tendency towards magnetic ordering. Indeed, the extrapolated zero-temperature transition is second order. The extended dynamical mean field analysis turns out to be somewhat subtle. The Bose-Fermi Kondo model with Ising anisotropy and in the absence of a static local field has a quantum phase transition: while it is in a paramagnetic Kondo state when the coupling  $g$  to the bosonic bath is weak, the phase at large  $g$  contains a finite Curie constant [39]. Since the existence of a Curie constant is hard to see at high temperatures, it is important to reach sufficiently low temperatures in order to determine the nature of the zero-temperature phase transition, as was done in Ref. [30]. The continuous nature was not seen in a numerical study at higher temperatures [40].

The quantum Monte-Carlo access to the local quantum critical point also provides an opportunity to numerically determine the exponent  $\alpha$  defined in Eqs. (5,6). In the Ising case, it is found [31] to be approximately 0.72. Two observations about the fractional exponent are worth making. First, the exponent turns out to be nearly universal for this model: within the numerical accuracy, the value is the same for four different sets of initial parameters. Second, there is limitation to an analytic study based on a rotor  $O(N)$  generalization of the model [the physical case, studied in the numerical work, corresponds to  $N = 1$ ]. While it captures the local quantum criticality (destruction of the Kondo effect at the magnetic QCP), the rotor large- $N$  generalization, in either the leading order [31] in  $1/N$  or the next-to-leading order [41], fails to capture the fractional exponent shown in the  $N = 1$  case. This limitation is understood to be the result of a “pinning” of the critical amplitude of the local susceptibility in the large- $N$  limit [31].

### 3.2 Beyond microscopics

These results have been argued [4,29] to be robust beyond the microscopic approach, when the exponent  $\alpha$  is fractional. The key point is that, for the long-wavelength spin fluctuations, the dynamic exponent  $z = 2/\alpha$ . For  $\alpha < 1$ , it is internally consistent to have the spatial anomalous dimension  $\eta = 0$ . The temporal fluctuations, on the other hand, contain a large anomalous dimension reflecting the destruction of Kondo effect.

### 3.3 In what sense is the QCP local?

There are several ways to characterize the local nature of the QCP.

First, there is a localization of  $f$ -electrons at the QCP. On the paramagnetic side, the  $f$ -local moments are part of the low-energy electronic excitations<sup>1</sup>. This happens as a result of the Kondo effect: through the Kondo singlet formation, the local moments and conduction electrons are entangled and the initially charge-neutral  $f$ -moments are turned into charge- $e$  and spin- $\frac{1}{2}$  quasiparticle excitations. In other words, the  $f$ -moments behave essentially as delocalized electrons. Indeed, the Fermi surface is adiabatically connected to that of a system in which the  $f$ -electrons are simply taken as non-interacting electrons! In the case of one  $f$ -element per unit cell, the Fermi volume is proportional to  $1 + x$ , where 1 counts the  $f$ -local moment and  $x$  is the number of conduction electrons per unit cell. On the magnetically ordered side, on the other hand, the  $f$ -moments stay charge neutral and are not a part of the electron fluid. The Fermi surface is that of the conduction electrons alone, under the influence of a static and periodic magnetic field produced by the antiferromagnetic order parameter. Even in the paramagnetic Brillouin zone, the Fermi volume is proportional to  $x$ . The discontinuous reconstruction of the Fermi surface takes place precisely at the QCP; see Fig. 2. Exactly at the QCP, the effective electronic mass diverges over the *entire* Fermi surface.

Second, the local nature is also reflected in the magnetic dynamics. The same anomalous exponent in the frequency and temperature dependences appears essentially *everywhere* in the Brillouin zone. And the local spin susceptibility is singular.

Both characterizations are symptomatic of the embedding of the destruction of Kondo effect into the magnetic ordering transition. The non-Fermi liquid excitations, which arise when the weight of the Kondo resonance just goes to zero, are part of the quantum-critical spectrum. The critical theory must incorporate these non-Fermi liquid excitations, and so it is no longer just the  $(d + z)$ -dimensional fluctuations of the order parameter as in the paramagnon theory of the  $T = 0$  SDW transition.

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<sup>1</sup> Here we are concerned with the low-energy behavior. At high-energy atomic scales, there are no local moments and  $f$ -electrons are always a part of the electronic spectrum.

## 4 Experiments

### 4.1 Spin Dynamics

The local quantum critical point is an interacting fixed point, in contrast to the Gaussian fixed point of the paramagnon theory. This is directly manifested in the spin dynamics. The  $\omega/T$  scaling and fractional exponent of the dynamical spin susceptibility have, as mentioned earlier, already been found in  $\text{CeCu}_{6-x}\text{Au}_x$ . In addition, the spin self-energy shown in Eq. (5) yields a dynamical susceptibility of the form given in Eq. (2), with the same fractional exponent appearing in a broad region of the Brillouin zone. (Closely-related features in the dynamics [42,43] and thermodynamics [44] appear in the compound  $\text{UCu}_{5-x}\text{Pd}_x$ .)

The static bulk spin susceptibility is also expected to show the same fractional exponent<sup>2</sup>:

$$\chi(T) = \frac{1}{\Theta + BT^\alpha} \quad (7)$$

This was already seen in  $\text{CeCu}_{6-x}\text{Au}_x$  early on [22]. Within a more limited temperature range, a fractional exponent has also been observed in  $\text{YbRh}_2\text{Si}_2$  [45]. Eq. (7) is also compatible with the data [46,47] in the normal state of  $\text{CeCoIn}_5$ , although the extent to which this system is quantum critical remains to be established.

The NMR relaxation rate probes local spin dynamics, at a frequency that is much smaller than the typical measurement temperature. Assuming a featureless hyperfine-coupling, the relaxation rate was predicted to contain a temperature-independent component [4,29]:

$$\frac{1}{T_1} \sim A_{hf}^2 \frac{\pi}{8A} \quad (8)$$

This has been subsequently observed in the Si-site NMR relaxation rate of  $\text{YbRh}_2\text{Si}_2$  [48]. For  $\text{CeCu}_{6-x}\text{Au}_x$ , recent measurement [49] of the Cu-site NMR sees  $1/T_1 \sim T^\alpha$  instead. It seems that the only way this result can be compatible with the inelastic neutron-scattering data is to invoke a strongly momentum-dependent hyperfine coupling constant such that the NMR relaxation rate is dominated by contributions from generic wavevectors. If that is indeed the case, the NMR experiment would provide additional evidence that the very same fractional exponent appears at generic wavevectors.

### 4.2 Thermodynamics

A divergent specific heat coefficient (specific heat divided by temperature) at the QCP is expected from the localization of the  $f$ -electrons: the effective

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<sup>2</sup> If the total spin is conserved, the spin conservation law may modify the behavior of the susceptibility near  $\mathbf{q} = \mathbf{0}$ .



mass diverges over the entire Fermi surface, as mentioned earlier. However, a divergent specific heat coefficient can also arise in some special cases [50] of the SDW quantum critical point, due to contributions of the so-called “hot spots” alone.

A more definite probe turns out to come from thermodynamic ratios. Recall that, at classical critical points, thermodynamic quantities such as specific heat diverge and provide the means to measure scaling exponents. Since a QCP occurs at zero-temperature, the third-law of thermodynamics dictates that the specific heat has to go to zero. On the other hand, thermodynamic ratios can still diverge. A practical example is the Grüneisen ratio – the ratio of the thermal expansion,  $\alpha \equiv \frac{1}{V} \frac{\partial V}{\partial T}$ , to the specific heat,  $c_p$ :

$$\Gamma = \frac{\alpha}{c_p} \sim \frac{\partial S / \partial p}{T \partial S / \partial T}. \quad (9)$$

Under scaling, this ratio must diverge at a QCP [51]. Moreover, the Grüneisen temperature exponent  $x$ , as defined by  $\Gamma_{\text{crit}}(T) \sim 1/T^x$ , measures the scaling dimension of the most singular operator coupled to pressure. It turns out that, within the paramagnon theory of an antiferromagnetic SDW transition,  $x$  is equal to 1 (up to logarithmic corrections in some cases). At a local quantum critical point, on the other hand,  $x$  can be fractional.

This divergence has now been observed experimentally [52] in two heavy fermion compounds,  $\text{YbRh}_2\text{Si}_2$  and  $\text{CeNi}_2\text{Ge}_2$ . For  $\text{CeNi}_2\text{Ge}_2$ , the Grüneisen temperature exponent is found to be equal to 1. For  $\text{YbRh}_2\text{Si}_2$ , it is fractional and is approximately 0.7 – this value is inconsistent with the paramagnon theory but is compatible with the scaling dimension (0.66 to the second order of the  $\epsilon$ -expansion) of the operator that tunes the system to local quantum criticality.

### 4.3 Electronic Measurements

The dynamical and thermodynamic measurements provide compelling evidence for the breakdown of the paramagnon theory in some of the heavy fermion metals, and make a strong case for the local quantum critical picture. Ultimately, one would like to test the destruction of the Kondo effect directly, and this can only be done through electronic measurements. Such evidence is just emerging, from for example the recent Hall measurements [53].

## 5 Broader context

Heavy fermions represent a prototype strongly correlated system to study quantum critical physics. It is simpler than the doped Mott insulators in that a large separation of energy scales exists: the local-moments are well defined over a broad energy range, and the Kondo coupling is much smaller than both the bare conduction electron bandwidth and the atomic Coulomb

interactions. It nonetheless is similar to the Mott-Hubbard systems in that the strong Coulomb interactions lead to a microscopic Coulomb blockade. The resulting projection of Hilbert space is essential to the destruction of the Kondo effect and the concomitant non-Fermi liquid excitations. This raises the prospect that an inherent interplay between non-Fermi liquid and quantum critical physics takes place in other strongly correlated electron systems as well: for high temperature superconductors, such considerations are in line with the scaling behavior observed near the optimal doping.

It is also instructive to relate the quantum critical metal physics with some recent work on quantum critical magnets [15]. The transition considered in the Kondo lattice and that in the quantum magnet are different: in the former it is between a paramagnetic metal and an antiferromagnetic metal and there is a well-defined order parameter only on one side; in the latter the transition considered is between a “valence-bond solid” and an antiferromagnetic insulator, both of which break translational symmetry and each has its distinct order parameter. Nonetheless, there are parallels between the two cases:

- The non-Fermi liquid excitations of a Kondo lattice  $\longleftrightarrow$  the fractionalized spin excitations – “spinons” – of a quantum magnet.
- The Kondo singlets – formed between the local moments and conduction electrons – of a Kondo lattice  $\longleftrightarrow$  the valence bond – or spin singlets formed between the local moments across bonds – of a quantum magnet.
- The Kondo singlet formation in the ground state implies conventional Kondo resonances – spin- $\frac{1}{2}$  and charge- $e$  Landau quasiparticles – in the excitation spectrum of a Kondo lattice  $\longleftrightarrow$  the valence bond formation in the ground state is symptomatic of the confinement of spinons in a quantum magnet.
- The destruction of the Kondo singlet is responsible for the emergence of the non-Fermi liquid excitations at the QCP of a Kondo lattice  $\longleftrightarrow$  the destruction of the valence bond is responsible for the emergence of spinons that are not confined at the QCP of a quantum magnet.
- The non-Fermi liquid excitations and the spinons in a Kondo lattice and a quantum magnet, respectively, are a part of their respective quantum-critical spectrum.
- In both cases, the excitations of the two phases that the QCP separates are conventional.

These parallels arise in spite of the differences in the model and in the underlying physics. They suggest the exciting possibility that a breakdown of the fluctuating order parameter theory occurs over a wide range of strongly correlated systems.

## 6 Summary

We have described some recent developments in the area of quantum critical metals, with an emphasis on the interplay between non-Fermi liquid physics and quantum critical behavior. In addition to the traditional consideration that quantum criticality leads to non-Fermi liquid behavior, the new realization is that the non-Fermi liquid excitations should be treated as part of the quantum-critical theory thereby leading to new classes of quantum phase transitions.

In the specific case of quantum critical heavy fermions, the non-Fermi liquid physics is characterized by a destruction of the Kondo effect. This results in the picture of local quantum criticality. Experimental evidence for this picture has come from inelastic neutron scattering, NMR, Grüneisen ratio, and Hall effect.

Finally, general considerations and specific examples suggest that the breakdown of the order parameter fluctuation theory and the emergence of novel excitations at a quantum critical point are properties relevant to a broad range of strongly correlated matters.

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